"MOLECULAR INTERACTIONS AND RELAXATION STUDIES OF ACETATE USING BROADBAND DIELECTRIC SPECTROSCOPY"

Synopsis

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By

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Abstract of Proposed Work Plan/Problem

"MOLECULAR INTERACTIONS AND RELAXATION STUDIES OF ACETATE USING BROAD BAND DIELECTRIC SPECTROSCOPY"

1. Introduction

An intermolecular force (IMF) is the force that mediates interaction between molecules, including the electromagnetic force of attraction or repulsion which act between atoms and other types of neighboring particles, e.g., atoms or ions [1]. Intermolecular forces determine bulk properties, such as the melting points of solids and the boiling points of liquids. These forces are electrostatic in nature; that is, they arise from the interaction between positively and negatively charged species. Like covalent and ionic bonds, intermolecular interactions are the sum of both attractive and repulsive components. Because electrostatic interactions fall off rapidly with increasing distance between molecules, intermolecular interactions are most important for solids and liquids, where the molecules are close together [2].

Hydrogen bonding refers to the formation of hydrogen bonds, which are a special class of attractive intermolecular forces that arise due to the dipole-dipole interaction between a hydrogen atom that is bonded to a highly electronegative atom and another highly electronegative atom which lies in the vicinity of the hydrogen atom. For e.g., in water molecules (H_2O), hydrogen is covalently bonded to the more electronegative oxygen atom. Therefore, hydrogen bonding arises in water molecules due to the dipole-dipole interactions between the hydrogen atom of one water molecule and the oxygen atom of another H_2O molecule [3].

For present study acetate is used as solute. An Acetate are class or category of chemical compound that contain methyl group(-ch_3) which is bounded with carbonyl carbon, the carbonyl group is connected to another oxygen (negative charge) with methyl group. Mainly,

acetate (Ethyl Acetate) is a polar solvent due to the presence of polar carbon oxygen bond, it can still however dissolve in non-polar compound since it has alkyl group which are non-polar in nature [4]. The main interest of study to understand dielectric properties of acetate insolvent like 1,4 - Dioxane.

Time Domain Dielectric relaxation spectroscopy is one of the most popular spectroscopies having frequency range from 10^{-4} Hz to 10^{12}Hz. So, this spectroscopy is known as broadband dielectric spectroscopy. The Broadband dielectric spectroscopy has very sensitive relaxation process for an extremely wide range of time i.e., $10^{5} – 10^{-12}$(seconds).This technique covers a broadband of frequencies in a single measurement. Considerable dielectric relaxation work has been done in our laboratory on diol– water mixtures using time domain reflectometry and also useful to study dielectric relaxation parameters of liquids. Dielectric spectroscopy is used to understand the various terms like interaction between solute –solvent, charge distribution, orientation of molecules [5-11].

Purpose of present work is to study dielectric relaxation and structural and dynamic behavior of acetates in solvent like 1,4 - Dioxane using BDS technique. Broadband Dielectric Spectroscopy (BDS) measurement technique will be used to study the various properties of acetates, also used to determine the dielectric properties of the material such as Static dielectric constant (ε0), dielectric constant (ε,), dielectric loss (ε”) and dielectric Relaxation time(τ).

2. Literature Review and Development in the Subject (previous work done in the relevant area):

Debye (1927) established that dielectric relaxation, which is the dispersion of the real permittivity (ε′) and the occurrence of dielectric absorption (ε″) in the domain for dipolar liquids and solids, was due to the reorientation motions of the molecular dipoles. Smyth (Princeton) and Cole (Brown) were started in the 1930s [13]. Prior to the 1950's many physicists aimed to model and measure the dielectric response of small molecules in the gas and liquid phase.There are number of investigations is carried out in last two decades on acetate by using various spectroscopic techniques in the presence of polar and non-polar solvent to understand the orientation of electric dipoles, electric dipole density in the mixture, dielectric properties and thermodynamic properties of the mixture [14-21].R.M. Shirke at.al.Studied the temperature dependent dielectric relaxation study of acetate-Alcohol mixtures using time domain technique in the frequency range 10 MHz to 20 GHz to understand the intermolecular interaction in the mixture [14-15].S.S. Birajdar at.al. S.S. Birajdar at.al. Investigated the structural and molecular dynamics of methyl acetate-xylene solutions using dielectric relaxation spectroscopy [16].

3. Objective of research/Proposed Hypothesis:

To carry out dielectric measurements of acetate solutions using time domain dielectric relaxation spectroscopy technique having frequency range 10MHz to 50GHz at different temperature for following systems.

(i) Methyl Acetate

(ii) Ethyl Acetate

(iii) Iso-propyl Acetate

(iv) N-butyl Acetate

(v) Amyl Acetate

Therefore, present objective of the work is to study the Acetate solutions and determine the following parameters:

- To determine complex permittivity of Acetate using Time Domain Reflectometry Technique.
- To determine static dielectric constant, dielectric loss and relaxation time at high frequency.
- To determine the Excess dielectric Permittivity.
- To study molecular interaction and hydrogen bonding of solvents through various parameters like Kirkwood correlation factor, Bruggeman factor, Thermodynamic Parameters, Excess parameters etc. using picoseconds dielectric relaxation spectroscopy.

4. Methodology to be adopted:

Time Domain Reflectometry (TDR) technique is very much useful for measurement of complex permittivity spectra in broad range of frequencies in single measurement. The Tektronix model no. DSA8300 Digital Serial Analyzer sampling mainframe along with the sampling module will be used for the time domain reflectometer (TDR). Figure 1 shows experimental setup for TDR[22-23]. A repetitive fast rising 250mV voltage pulse of 200 KHz with 12ps incident and 15ps reflected rise time was fed through coaxial line system of impedance 50 ohm. Sampling oscilloscope monitors changes in step pulse after reflection from the end of line. Reflected pulse without sample R1(t) and with sample Rx(t) will be recorded in time window of 5ns and digitized in 2000 points [23].

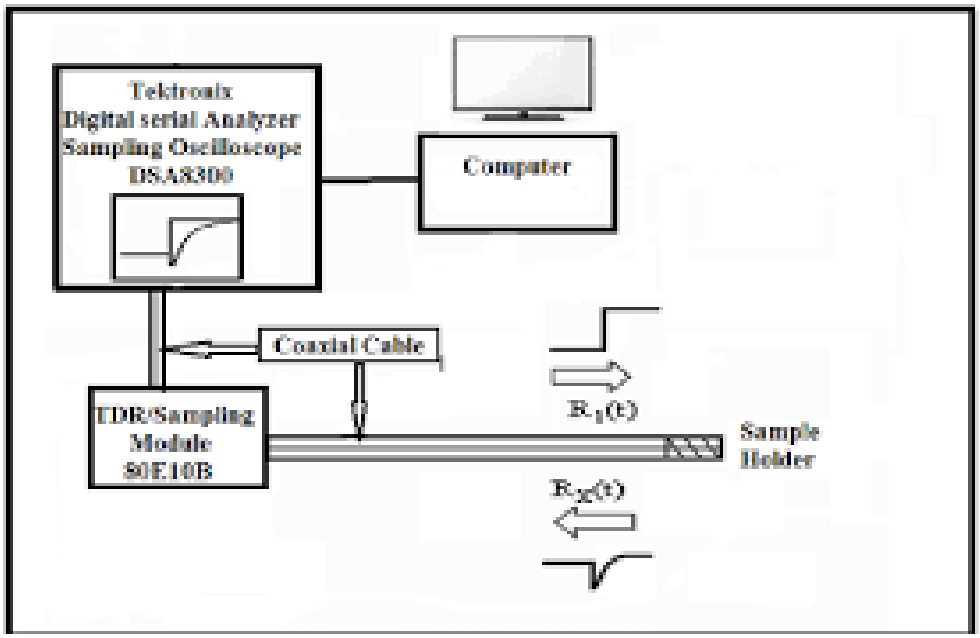

Fig1. Block diagram of Time Domain Reflectometry.

5. Importance of study/society application:

In recent years, dielectric measurements have become an effective tool for extracting significant information related to the structure and to the quality-status of various material.

- **International/National status:**The following scientist are actively doing research in this field at international/National level:

1. Dr. Richard BuchnerInstitute for Physical and Theoretical Chemistry, University of Regensburg, Regensburg, Germany.
2. Dr. Bahrpaima, Department of Chemistry, Guilan University, Rasht, Iran
3. Dr. Zhuravlev V.I., Department of Chemistry, Moscow State University, Moscow, Russia.
4. R.J. Sengwa, Jodhpur, JNV University, Jodhpur (RS).
5. Dr. G. Arivazhagan,Dept. of Physics, Thiagarajar College, Teppakulam, Madurai

- **Significance of the study:**

Dielectric spectroscopy of associating liquids offers valuable insights into the micro dynamics of fluctuating hydrogen bonded liquids. It has various application in various fields. The present study is devoted to dielectric relaxation of Acetate in solvent like 1,4 Dioxane using TDR technique from 10MHz to 30GHz. from dielectric relaxation parameters; and understand orientation through solute-solvent interactions.

6. **Proposed work plan/Formulation and structure of study:**

1. **First Year:**

   (i) Literature survey on acetate and related to the topic

   (ii) Coursework as per university syllabus,

   (iii) Literature Review system to be studied.

2. **Second Year:** Study of Dielectric measurement of Acetate and determine the dielectric parameters such as static dielectric constant, relaxation time, dielectric constant at high frequency and Kirkwood correlation factor.

3. **Third year:**

   a. Paper presentation in the International/National Conference.

   b. Writing research Paper and publish paper in the International Journals.

   c. Thesis Writing and submission.

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